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A PARAMETRIC DESCRIPTION OF A SKEWED PUFF IN THE DIABATIC SURFACE LAYER

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Abstract. The spreading of passive material in the stable, neutral and unstable surface layer from an instantaneous ground source is parameterized in a form appropriate for use with an operational puff diffusion model.

INIS descriptors: AIR POLLUTION; CLUSTER EMMISSION MODEL; DIFFUSION; GAUSSIAN PROCESSES; NUMERICAL SOLUTION; PLUMES; POLLUTANTS; RADIOACTIVE CLOUDS; SPATIAL DISTRIBUTION; SURFACE AIR

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CONTENTS

1. INTRODUCTION

Spatial and temporal variations in meteorological conditions, including nonuniform topographical features, lake or sea-breeze circulation, and urban heat-island effects have during the past years given basis for the proposal of several puff diffusion models: Roberts et al. (1970), Lamb and Neiburger (1971), Start and Wendell (1974), Ludwig et al. (1977), Shieh (1978), Mikkelsen (1979) and Mikkelsen et al. (1980). The release of pollutant from the source are here treated as a series of puffs emitted successively into the atmosphere. The concentration distribution of the individual puffs have hitherto been assumed to be Gaussian along the vertical as well as along the horizontal axes. The model of Shieh (1978), however, included also the effect of wind shear and buoyant plume rise.

In analogy to diffusion from a continuous source, specifically the vertical diffusion from an instantaneous source is strongly influenced by the effect of atmospheric stability. This applies with respect to the spreading of the cloud and with respect to the shape of the vertical distribution function as well.

Therefore, an operational puff model algorithm is here proposed which takes into account the effect of stability: 1) on the vertical dispersion of the cloud, 2) on the shape of the vertical concentration distribution and 3) on the wind shear induced spread.

2. THEORY

2.1. Parameterization of vertical puff diffusion

By assuming identity of eddy diffusivities of passive material K_z and of heat K_h, Chaudhry and Meroney (1973) studied the effect of stability on the instantaneous vertical diffusion from a ground level point source. Nieuwstad and van Ulden (1978) showed that this identification could lead to an overprediction of the vertical spread from a continuous source in stable conditions and obtained better agreement with the Prairie Grass data with $K_z = \alpha_o K_m$, where K_m is the eddy diffusivity for momentum, and α_o is a constant which is equal to the ratio K_h/K_m in neutral stratification. In the present model K_z is set equal to K_h, but with the remark above in mind, later experimental findings may make a change to $\alpha_o K_m$ appropriate. This, however, will from a mathematical point of view only amount to a trivial substitution.

The Lagrangian similarity hypothesis considers the problem of diffusion of an ensemble of marked particles of fluid, released individually from a fixed ground source at time $t = 0$. Each such released fluid particle will occupy a different position at time t after the release, and $\bar{X}(t)$ and $\bar{Z}(t)$ denotes the average longitudinal and vertical displacements of the ensemble from the source position, at time t. In a homogeneous and stationary flow field, such a diffusion may be like that of a cloud of marked particles or a puff, released from a ground source at one instant (Pasquill, 1966), see Fig. 1. Consequently, the distribution of concentration $C(x,y,z,t)$ [kg m^{-3}] at a point (x,y,z) at time t in a cloud of passive substance may be described by the diffusion equation in a plane homogeneous turbulent shear layer

$$\frac{\partial C}{\partial t} + \bar{u}(z)\frac{\partial C}{\partial x} = \frac{\partial}{\partial z}\left(K_z \frac{\partial C}{\partial z}\right) + \frac{\partial}{\partial y}\left(K_y \frac{\partial C}{\partial y}\right) . \qquad (2.1)$$

The longitudinal diffusion term is neglected, this being much smaller than the corresponding term $\bar{u}(\partial C/\partial x)$. K_y and K_z are the eddy diffusivities of matter in the y and the z directions, respectively. The downwind direction is denoted by x and $\bar{u}(z)$ is the mean wind speed as function of height z. C's dependence of y in the above equation can be integrated out to give

$$\frac{\partial \tilde{C}}{\partial t} + \bar{u}(z)\frac{\partial \tilde{C}}{\partial x} = \frac{\partial}{\partial z}\left(K_z \frac{\partial \tilde{C}}{\partial z}\right) \tag{2.2}$$

where $\tilde{C}(x,z,t) = \int_{-\infty}^{\infty} C(x,y,z,t)dy$ [kg m^{-2}] is the concentration that would arise from an infinitely long, crosswind oriented line source. If the total amount of substance in the cloud is unity, the instantaneous position of its centre of mass coordinate will be given by

$$\bar{x}(t) = \int_{-\infty}^{\infty} x \, \tilde{C}(x,z,t) \; dxdz \tag{2.3}$$

$$\bar{z}(t) = \int_{0}^{\infty} z \, \tilde{C}(x,z,t) \; dxdz \tag{2.4}$$

Multiplying Eq. (2.2) by z and x, respectively, a subsequent integration over all values of x and z yields for times t > 0

$$\frac{d\bar{z}}{dt} = \int_{0}^{\infty} z\frac{\partial}{\partial z}\left(K_z \frac{\partial C_y}{\partial z}\right)dz \tag{2.5}$$

$$\frac{d\bar{x}}{dt} = \int_{-\infty}^{\infty} u(z) \; C_y \; dz \tag{2.6}$$

where $C_y = \int_{-\infty}^{\infty} \tilde{C}\ (x,z,t)\ dx$ [kg m^{-1}] denotes the average concentration of particles in the x-y plane at height z, (see again Fig. 1). An equation for the distribution of C_y in the vertical can be obtained by integrating Eq. (2.2) with respect to x, as

$$\frac{\partial C_y}{\partial t} = \frac{\partial}{\partial z}\left(K_z \frac{\partial C_y}{\partial z}\right) \tag{2.7}$$

The important relationship in Eq. (2.5) and (2.6) for the centre of mass coordinates of the puff can now be evaluated for termally stratified flow if $K_z(z)$ and $C_y(z,t)$ are known. Using the Monin-Obukhov similarity hypothesis yields the relation

$$K_z = \frac{k\ u_* z}{\phi_h(\frac{z}{L})} \tag{2.8}$$

where k is von Karman's constant (0.35), u_* the friction velocity and $\phi_h(z/L)$ is the dimensionless temperature gradient, which is a function of the ratio between the height z and the Monin-Obukhov length L, only.

The diffusion equation (2.7) can be solved analytically when this eddy diffusivity is approximated by a power-law profile $K_z = K_1\ z^n$. For such a profile the solution of Eq. (2.7) is (Sutton, 1953)

$$C_y = \frac{a}{\bar{z}} \exp[-\ (bz/\bar{z})^q]\quad , \tag{2.9}$$

where

$$q = 2-n$$
$$a = q\Gamma(2/q)/\Gamma^2(1/q)$$
$$b = \Gamma(2/q)/\Gamma(1/q),$$

and where Γ is the Gamma function. The power n may be regarded as an index of stability. Estimates for n and for $q = 2-n$ can be obtained by a procedure suggested by Klug (1963) to fit a power law representation to the original K_z-profile. This procedure yields

$$n = \{d\log K_z/d\log z\}_{z=\bar{z}} \qquad (2.10)$$

From Businger (1973) is taken

$$\phi_h = 0.74(1 + 6.3\ z/L) \qquad \text{for } 1/L \geq 0 \qquad (2.11)$$

and

$$\phi_h = 0.74(1 - 9\ z/L)^{-1/2} \qquad \text{for } 1/L \leq 0 \qquad (2.12)$$

The corresponding powers obtained on the basis of Eq. (2.9) and with $q = 2-n$ are

$$q = \frac{0.74}{0.74+4.7\ \bar{z}/L} \qquad \text{for } 1/L \geq 0 \qquad (2.13)$$

$$q = \frac{1-13.5\ \bar{z}/L}{1-9\ \bar{z}/L} \qquad \text{for } 1/L \leq 0 \qquad (2.14)$$

For neutral conditions $q = n = 1$, whereby the puffs vertical distribution function simply becomes

$$C_V = \frac{1}{\bar{z}} \exp[-z/\bar{z}] \tag{2.15}$$

This enlightens the important difference between a continuous released plume and an instantaneous puff. In contrast to the result in Eq. (2.15), dispersion from a continuous ground level source, obtained from measurements at a fixed point in space, typically fits to the power $q \approx 1.3$ under neutral conditions.

For a limited range of the stability index q around 1, Chaudhry and Meroney (1973) reduced the expressions on the right hand side of Eq. (2.5) and Eq. (2.6), to the approximative form, which will be used in the following

$$\frac{d\bar{z}}{dt} \approx k u_* \phi_h^{-1}(\bar{z}/L) \tag{2.16}$$

and

$$\frac{d\bar{x}}{dt} \approx \bar{u}(\bar{z}) - 1.44\, u_* \tag{2.17}$$

The mean wind speed over local homogeneous terrain, as function of height z, is here also taken from Businger (1973)

$$\bar{u}(z) = (u_*/k)\left[\ell n(z/z_o) - \Psi(z/L)\right] \tag{2.18}$$

where, for $1/L \geq 0$

$$\Psi = -4.7\, z/L \tag{2.19}$$

and for $1/L \leq 0$

$$\Psi = 2\ln[(1+x)/2] + \ln[(1+x^2)/2] - 2\tan^{-1}(x) + \pi/2 \qquad (2.20)$$
$$x = (1 - 15\,z/L)^{1/4}$$

The individual released puffs, however, must be advected, not by the mean wind $\bar{U}$, but by the non-stationary wind field $\underline{V}$, which in general is a function of the downwind position x, the time since releases t, and the wind field averaging time t_{av}. For use with microscale and mesoscale puff models, the wind field $\underline{V}$ is obtainable by an "objective" wind field analysis, based on simultaneous measurements of wind speed and directions from a network of meteorological towers (see e.g. L.L. Wendell, 1970). Dependinj on the size of the puffs, the averaging time t_{av}, (which also conveniently is used in computer simulations as the basic time step for the puff advection), must be short enough to ensure that sufficient temporal variation will remain in the flow field.

If $\bar{u}(z_m)$ represents the speed of the wind vector $|\underline{V}|$ during the time interval from t to t + t_{av}, at the height z_m and at the horizontal position (x,y,z), then the wind-speed for advection of the puffs in that horizontal position, and over the time period from t to t + t_{av} is calculated by means of

$$\bar{u}_r(z) = \bar{u}(z_m) \cdot \left[\frac{\ln(z/z_o - \Psi(z/L)}{\ln(z_m/z_o - \Psi(z_m/L)}\right] , \qquad (2.21)$$

assuming that $|\underline{V}|$ also follows the usual mean wind profile. For use with an operational puff diffusion algorithm, the set of equations (2.9), (2.16) and (2.17), determines together with the wind field in Eq. (2.21) the shape of the puffs vertical distribution function as well as their downwind position as function of stability and travel time. Nevertheless, these equations are based on the approximations. It is assumed that K_z can be represented by a power law of the variable z, and therefore their validity must be based on a comparison with a numerical solution of the diffusion equation (2.7) with the eddy diffusivity K_z as specified by the equations (2.8) and (2.11).

2.2. Numerical solutions

The boundary conditions applied to a numerical solution of the diffusion equation (2.7) is

$$K_z \frac{\partial C_y}{\partial z} = 0 \text{ for } z = z_0 \tag{2.22}$$

and

$$K_z \frac{\partial C_y}{\partial z} = 0 \text{ for } z \to \infty \quad .$$

They state that the mass flux to the ground and the mass flux for large values of z must vanish. The initial vertical concentration distribution function was chosen to be Gaussian with maximum concentration at ground level and a standard deviation equal to $2z_0$. Except for very small values of the dimensionless time u_*t/L, the numerical results were found to be insensitive to the specific form of the initial distribution.

With the boundary and initial conditions as described, the diffusion equation in non-dimensional form

$$\frac{\partial C_y}{d(u_*t/L)} = k \frac{\partial}{\partial \eta} (\eta \phi_h^{-1}(\eta) \frac{\partial C_y}{\partial \eta}), \tag{2.24}$$

where $\eta = z/L$, was solved numerically by a finite difference scheme proposed by Keller (1971) and implemented for use in the investigations by S.E. Gryning et al. (1982). During numerical calculations, the conservation of mass was continuously verified by integration of the flux of material in the vertical direction. As also found by Gryning et al. (1982), errors were maintained below 1%.

2.3. Results

Comparison were made between the numerical solutions of Eq. (2.24) and the approximation suggested in section 2.1. Fig. 2 compares the variation of the mean height of the puff $\bar{z}$ as function of the puffs travel time $u_*t/|L|$. The suggested approximation in Eq. (2.16) is seen to model very well the variation of $\bar{z}$ based on the numerical integration of the diffusion equation, together with the definition of $\bar{z}$ in Eq. (2.4).

In the limit for small times $tu_*/|L| \to 0$, which for fixed t corresponds to near neutral stratification, the approximate solution is $\bar{z} = ku_*t$. Based on the ϕ_h-functions chosen in Eq. (2.11) and (2.12) the asymptotic values for the large time limits are, for the stable and the unstable stratification, respectively: $\bar{z} \propto t^{1/2}$ and $\bar{z} \propto t^2$. Dimensional analysis for the z-less (very stable) stratification yields accordingly $\bar{z} \propto t^{1/2}$, but in the unstable atmosphere, for which case convective scaling applies and $\phi_h \approx (z/|L|)^{-1/3}$, dimensional analysis yields $\bar{z} \propto t^{3/2}$. The different asymptotic form found here, $\bar{z} \propto t^2$, results as a consequence of the empirical functional form observed for ϕ_h (Eq. (2.12)) in the convective limit. This discrepancy is deemed to be insignificant except under the most unstable conditions, in which case K-theory is known to be inapplicable under all circumstances.

Fig. 3 shows the shape factor q as function of the non-dimensional travel time of the cloud u_*t/L. The dots were obtained by least square fitting to the analytical function described by Eq. (2.9) of the vertical concentration profiles, obtained from the numerical solution of Eq. (2.24). The fittings was accomplished from the ground up to the level where the concentration constituted 5% of the maximum concentration by forcing the analytical function through the concentration at ground level. The relative root-mean-square difference turned out to be lower than 0.1% for the parameter interval $u_*t/|L| < 10^{-2}$. Under stable conditions the maximum error, of the order ~ 2%, was found for $u_*t/L = 5 \cdot 10^{-1}$. Correspondingly, the maximum error under unstable conditions was of the order 3% and was found with $u_*t/L = -5 \cdot 10^{-1}$. The very low root-mean-square error found for $u_*t/|L| < 10^{-2}$ reveals the fact that an exponential distribution function is an exact solution to the diffusion equation under neutral conditions, since n and hence q in Eq. (2.9) equals unity, when $1/|L| \sim 0$. The curve in Fig. 3 shows the analytical approximation suggested in Eq. (2.13) for stable and in Eq. (2.14) for unstable conditions.

For all practical purposes, these curves are found to represent the numerical solution very well. The variation in the shape parameter with travel time is quite pronounced. Under stable conditions, the initially small, exponential distributed cloud ultimatively becomes Gaussian, i.e. q = 2. Under unstable conditions, on the other hand, the ultimate vertical distribution function becomes quite streched ($q \approx 0.5$). This result shows a significant difference from the Gaussian vertical distribution usually assumed with puff-models.

3. THE MODEL

3.1. Horizontal puff diffusion

So far have exclusively being dealt with the particles vertical distribution function, which in the previous paragraph was defined as

$$C_V(z) = \iint_{-\infty}^{\infty} C(x,y,z)\, dxdy \qquad (3.1)$$

In order to calculate the entire concentration field C(x,y,z), however, also the distribution function of particles in the two horizontal directions have to be resolved. We therefore consider the part of the cloud which is confined to the small vertical interval Δz, centered about the horizontal plane $z = h$. The particles horizontal distribution function at this height C_H, is then, when normalized, given by the expression

$$C_H(x,y,h) = C(x,y,h)\Delta z / \iint_{-\infty}^{\infty} C(x,y,h)\Delta z \; dxdy \tag{3.2}$$

Thereby, also the mean horizontal positions, $\bar{x}$ and $\bar{y}$ of the particles in the small interval Δz about $z = h$ is given as

$$x_h = \iint_{-\infty}^{\infty} x \; C_H(x,y,h) \; dxdy \tag{3.3}$$

$$y_h = \iint_{-\infty}^{\infty} y \; C_H(x,y,h) \; dxdy \tag{3.4}$$

In contrast to dispersion taking place in the vertical direction in the atmosphere, horizontal dispersion of a cloud can, with some justification, be claimed to proceed in a homogeneous field of turbulence. This is true at least as long as the horizontal extent of the individual puffs, (but not the entire plume) is small compared to the inhomogeneity of the turbulent field. In this case, the ensemble averaged horizontal distribution function of the cloud is well taken to be Gaussian, both from theoretical considerations (e.g. Batchelor (1952)) and also from experimental evidence (e.g. Sullivan (1971)). Also Yang and Meroney (1972, 1973) measured at fixed x and z, the centerline concentration as function of time from a surface released cloud in a wind tunnel boundary layer. Wilson (1981) compared their measured skewed distribution with a Gaussian distribution and concluded that the errors induced by applying a symmetric Gaussian distribution to the along-wind diffusion (at fixed height) could be expected to be small compared with the uncertainties in estimating the corresponding along-wind standard deviation σ_x.

In the following reference will be changed from the fixed (absolute) coordinate system (x,y,z) to the frame of reference $(x_{z=0}, y_{z=0}, 0)$ moving with the centeroid of the cloud at height $z = 0$. In this moving frame we define a relative Cartesian coordinate system as

$$\begin{aligned} \tilde{x} &= x - \bar{x}_{z=0} \\ \tilde{y} &= y - \bar{y}_{z=0} \\ \tilde{z} &= z \end{aligned} \tag{3.4}$$

The mean horizontal position of the particles at the height z in this relative frame is also defined as

$$\begin{aligned} \tilde{\bar{x}}_z &= \bar{x}_z - \bar{x}_{z=0} \\ \tilde{\bar{y}}_z &= \bar{y}_z - \bar{y}_{z=0} \end{aligned} \tag{3.5}$$

In this relative frame of reference, an assumed horizontal Gaussian particle distribution function simply reads

$$C_H(\tilde{x},\tilde{y},\tilde{z}) = \frac{1}{2\pi\sigma_x\sigma_y} \exp\{-\tfrac{1}{2}(\tilde{x}-\tilde{\bar{x}}_z)^2/\sigma_x^2 - \tfrac{1}{2}(\tilde{y}-\tilde{\bar{y}}_z)^2/\sigma_y^2\} \tag{3.6}$$

where σ_x and σ_y are the streamwise and the lateral standard deviations, respectively, of the cloud at the fixed height z=h.

Suppose now that σ_x, σ_y, $\tilde{\tilde{x}}_z$ and $\tilde{\tilde{y}}_z$ are known functions of height z and time t. Then, as a consequence of the assumed form of the horizontal distribution function Eq. (3.6), the entire three-dimensional concentration field of the cloud must be given by

$$C(\tilde{x},\tilde{y},\tilde{z}) = C_V(\tilde{z}) \cdot C_H(\tilde{x},\tilde{y},\tilde{z}) \qquad (3.7)$$

Note that the marginal distribution C_V simply is retrived by integrating the right hand side over a horizontal plane.

3.2. Horizontal turbulent spread, σ_x and σ_y

In past dispersion studies (e.g. Pasquill, 1974) plume and puffs have shown different dispersion characteristics. While the spread of a plume as measured by the horizontal standard diviation of the concentration distribution initially tends to grow proportional to the downwind distance x, and ultimatively proportional to the square root of this distance, the characteristics of puff dispersion have shown a different behaviour. In particular, Gifford (1957) found by examining data from smoke puffs the existence of two predicted (Batchelor, 1952) growing regimes for the puffs lateral standard diviation σ_y. Initially, σ_y was found to increase proportional to x but then follows an intermediate regime, where σ_y grows proportional to the 3/2 power of the downwind distance. Ultimatively, when the lateral extent of the puff becomes large relative to the lateral length scale of the turbulence, the spread of a puff and a plume becomes identical. In contrast to dispersion characteristics available for plumes under various atmospheric conditions, corresponding formulas for puff growth are still relatively sparse.

For use within the atmospheric surface layer and for downwind distances not exceeding, 5000 meters say, Pasquill (1974) suggested the following expression, supported by the theory of

Smith and Hay (1961)

$$\sigma_y = 0.22ix \tag{3.8}$$

where i is the intensity of the turbulence, defined as $i = (\overline{u'^2} + \overline{v'^2} + \overline{w'^2})^{1/2}/\bar{u}$. As a practical working approximation, i is estimated from the crosswind eddy velocity, $\overline{v'^2}$, only. The quantity $(\overline{v'^2})^{1/2}/\bar{u}$ is to a good approximation equal to the root mean square value of the angular response $i_\theta = (\overline{\theta'^2})^{1/2}$ of a sensitive vane. In his comparison, Pasquill (1974) found reasonably good experimental agreement with Eq. (3.8) by setting $i = 2i_\theta$ in neutral and unstable stratifications and $i = i_\theta$ in the most stable stratifications. It should be mentioned that the theoretical analysis by Chatwin (1968) leads to a puff expansion which close to the ground in a logarithmic surface layer profile reads $\sigma_x = 0.596\ u_*t/k$, applicable in the limit for large diffusion times. Setting $u_*/k = (\overline{u'^2})^{1/2}$ from Businger (1973) and $i = 3(\overline{u'^2})^{1/2}/\bar{u}$, this becomes almost equivalent to Eq. (3.8). Here, the spread σ_x is a function of the travel time t of the puff rather than a function of the downwind distance x as in Eq. (3.8). In the present model, use will be made of Eq. (3.8) at short distances because of its experimental validation. For diffusion in the troposphere at distances greater than about 5000 meters, the formula given by Gifford (1982) can be recommended

$$\Sigma_y^2 = T-(1-e^{-T}) - (c/2)(1-e^{-T})^2 \tag{3.9}$$

Here, $\Sigma_y^2 = \sigma_y^2/(2\overline{v'^2}t_L^2)$, $T = t/t_L$ and c is a constant close to unify (0.9955)*). The quantity t_L is the integral timescale of the turbulence. Note that both of these formulas (Eq. (3.8) and Eq. (3.9)) applies to lateral spread only, and are independent of height z. Further local horizontal homogeneity will be assumed together with the relation $\sigma_x = \sigma_y$ for fixed heights.

*) Reference is made to the original work (Gifford, 1982) for a more complete discussion.

3.3. Wind shear effect

As shown for instance by Chatwin (1968), the horizontal spread of a cloud is, except under the most unstable conditions, strongly influenced by the interaction of wind shear and vertical diffusivity. By assuming that the wind shear is approximatively constant across the cloud, we can, as also suggested by Sheih (1978), incorporate the shearing effect in the cloud by the relations

$$\bar{\tilde{x}}_z = \zeta\tilde{z} \tag{3.10}$$

and

$$\bar{\tilde{y}}_z = \xi\tilde{z} \tag{3.11}$$

The value of the variables ζ and ξ can be calculated by following the horizontal mean position of two tracer particles (1) and (2), displaced respectively above and below the mean height $\bar{z}(t)$ by the constant fraction F of the mean height of the cloud

$$F = (z_1 - z_2)/2\bar{z}. \tag{3.12}$$

Here, z_1 and z_2 are the vertical positon of the particles (1) and (2), respectively. With the two particles initially at the downwind position $x_1 = x_2 = 0$, the variable ζ which determines the alongwind shearing of the puff as function of time and stability, is calculated by (cf. Fig. 4)

$$\zeta = \frac{x_1 - x_2}{\bar{z}} = \frac{1}{\bar{z}} \int_0^t (\bar{u}_r\{\bar{z}(1+F)\} - \bar{u}_r\{\bar{z}(1-F)\})d\tau \tag{3.13}$$

Equivalently, the variable ξ determining the cross wind shearing of the puff is calculated by

$$\xi = \frac{y_1 - y_2}{\bar{z}} = \frac{1}{\bar{z}} \int_0^t \bar{v}_r\{\bar{z}(1+F)\} - \bar{v}_r\{\bar{z}(1-F)\}\, d\tau \qquad (3.14)$$

Analoguous, y_1 and y_2 are here the cross wind position of the two particles (1) and (2), and $v_r(z)$ is the short term averaged (averaging time = t_{av}, cf. Eq. 2.21) mean lateral windspeed as function of height.

In analogy to $\bar{u}_r(z)$, also $\bar{v}_r(z)$ is obtainable from the wind field $\underline{V}$ from an equation similar to Eq. (2.21), but in contrast to $\bar{u}_r(z)$ the mean value of $\bar{v}_r(z)$, averaged over many advection steps, is by definition equal to zero.

The only remaining parameter responsible for the shearing effect of the puff is the constant F. We will postpone the determination of this constant until we have investigated some statistical properties of the cloud's entire concentration distribution in the next section.

3.4. Statistical properties of the clouds distribution function

From the equations (3.4) and (3.5), the 3-dimensional particle distribution function of the skewed puff now reads

$$C(\tilde{x},\tilde{y},\tilde{z}) = \frac{a}{2\pi\sigma_x\sigma_y\,\bar{z}} \exp\{-\tfrac{1}{2}(\tilde{x}-\zeta\tilde{z})^2/\sigma_x^2) - \tfrac{1}{2}(\tilde{y}-\xi\tilde{z})^2/\sigma_y^2 - \left(\frac{b\tilde{z}}{\bar{z}}\right)^q\} \qquad (3.15)$$

With this distribution function given, it is relatively simple to derive the following statistical relations for the cloud

1) Center of mass

$$\tilde{\tilde{x}} = \zeta\bar{z} \qquad (3.16)$$

$$\tilde{\tilde{y}} = \xi\bar{z} \qquad (3.17)$$

2) Total horizontal variance, $\Sigma_x^2 \equiv \overline{x^2} - \bar{x}^2$ and $\Sigma_y^2 = \overline{y^2} - \bar{y}^2$

$$\Sigma_x^2 = \sigma_x^2 + \frac{\Gamma(\frac{1}{q})\Gamma(\frac{3}{q})-\Gamma^2(\frac{2}{q})}{\Gamma(\frac{2}{q})}\zeta^2\,\bar{z}^2 \qquad (3.18)$$

$$\Sigma_y^2 = \sigma_y^2 + \frac{\Gamma(\frac{1}{q})\Gamma(\frac{3}{q})-\Gamma(\frac{2}{q})}{\Gamma(\frac{2}{q})}\xi^2\,\bar{z}^2 \qquad (3.19)$$

3) Total vertical variance, $\Sigma_z^2 = \overline{z^2} - \bar{z}^2$

$$\Sigma_z^2 = \frac{\Gamma(\frac{1}{q})\Gamma(\frac{3}{q})-\Gamma(\frac{2}{q})}{\Gamma(\frac{2}{q})}\bar{z}^2 \qquad (3.20)$$

4) Correlation coefficient $\rho_{xz} \equiv \overline{xz}/\Sigma_x\Sigma_z$ and $\rho_{yz} = \overline{yz}/\Sigma_y\Sigma_z$

$$\rho_{xz} = 1/\{1 + \frac{\sigma_x^2}{(\Gamma_{123}-1)\zeta^2\bar{z}^2}\}^{\frac{1}{2}} \qquad (3.21)$$

$$\rho_{yz} = 1/\left\{1 + \frac{\sigma_y^2}{(\Gamma_{123}-1)\xi^2\bar{z}^2}\right\}^{1/2} \tag{3.22}$$

where $\Gamma_{123} \equiv \Gamma(1/q)\cdot\Gamma(3/q)/\Gamma^2(2/q)$. Note especially that for q=1 is $\Sigma_z^2 = \bar{z}^2$ and for q = 2 is $\Sigma_z^2 = (\frac{3}{2}\pi-1)\bar{z}^2$.

The correlation coefficients ρ_{xz} and ρ_{yz} have the properties that

$$\lim_{\zeta\to 0} \rho_{xz} = \lim_{\xi\to 0} \rho_{yz} = 0 \tag{3.24}$$

This corresponds to the case where no correlation exists between the particles position in the xz and the yz plane, respectively.

3.5. Determination of the shearing parameter, F

In order to calculate the variables (ζ,ξ) from Eq. (3.13) and (3.14), the shearing parameter F from Eq. (3.12) finally has to be determined. For a neutral atmosphere, Chatwin (1968) investigated theoretically the alongwind dispersion of a puff of passive contaminant, released from a source near the ground. He finds

$$\Sigma_x = 0.803 \quad \frac{u_* t}{k} \tag{3.25}$$

By setting q = 1 in Eq. (3.18), we have correspondingly for the skewed puff in a neutral atmosphere

$$\Sigma_x^2 = \sigma_x^2 + \zeta^2 z^2 \qquad (3.26)$$

Substitution of ζ from Eq. (3.13) herein gives

$$\Sigma_x^2 = \sigma_x^2 + [\int_0^t (u_r\{\bar{z}(1+F)\} - u_r\{\bar{z}(1-F)\})d\tau]^2 \qquad (3.27)$$

By use of the fact that the mean wind profile $u_r(z)$ is logarithmic in this neutral case, their result after integration

$$\Sigma_x^2 = \sigma_x^2 + \ln^2\{\frac{(1+F)}{(1-F)}\}\frac{u_*^2 t^2}{k^2} \qquad (3.28)$$

By estimation of σ_x^2 from Eq. (3.8) as $(0.22\ u\ t)^2$ and by substitution of Eq. (3.25) for Σ_x^2, F is determined from the following equation

$$(0.803)^2 = (0.22)^2 k^2 + \ln^2\{\frac{1+F}{1-F}\} \quad , \qquad (3.29)$$

from which we find F = 0.38.

The contribution to the total spread Σ_x from the spread at fixed height is, with the assumption $\sigma_x = 0.22\ u_* t$, indeed negligible relative to the contribution from the shearing of the puff $\ln\{(1+F)/(1-F)\}\ u_* t/k$ under neutral conditions.

Next turning to the case of a very stable atmosphere, where to a good approximation the wind shear $s = d\bar{u}_r/dz$ can be considered constant with height, the theory of Corrsin (1958) yields, for the shear induced spread in an unbound atmosphere

$$\Sigma_x^2 = \frac{1}{3} S^2 \Sigma_z^2 t^2 \qquad (3.30)$$

The previous case of a neutral atmosphere proved that σ_x was small relative to the contribution from the shearing of the puff. Since the shearing of the puff in the stable atmosphere is even more pronounced at the same time as the spread σ_x deminishes, we can neglict the contribution of σ_x^2 to Σ_x^2 in Eq. (3.27). From Eq. (3.18) and (3.20) we then approximately have that $\Sigma_x^2 = \zeta^2\Sigma_z^2$. For a very stable atmosphere we also have from Eq. (2.18) and (2.19) that $u_r(z) = 4.7\ u_*z/(kL)$ and hence $S = 4.7\ u_*/(kL)$. With this Eq. (3.13) becomes

$$\zeta = \frac{2FS}{\bar{z}(t)} \int_0^t \bar{z}(t')dt' \qquad (3.31)$$

In the very stable atmosphere we found that z(t) is proportional to $\sqrt{t}$, so in this case we have

$$\xi = \frac{4}{3}\ FSt \qquad (3.32)$$

The resulting streamwise spread of the skewed puff consequently becomes

$$\Sigma_x^2 = (\frac{4}{3}\ FS\Sigma_z t)^2 \qquad (3.33)$$

and comparison with Eq. (3.30) yields the value $F = 0.43$ to be compared with the previous result for the neutral case $F = 0.38$.

The slightly different values of the constant F found may be attributed to the following: Corrsin's model (Eq. 3.29) applies to the case of an unbound atmosphere, whereas Eq. (3.25) is for a ground level release. Consequently the vertical spread in the latter case is confined to the halfplane above ground level only. Turning finally to the case of a very unstable atmosphere, we expect the influence on Σ_x from the shearing of the puff to be negligible relative to the spread σ_x since the mean wind profile here is approximately constant with height and the parameter F is in this case left insignificant.

In conclusion, the above analysis suggest a value of the shearing parameter F close to 0.4 for use in models as a compromise for the broad range of stabilities discussed.

4. APPLICATIONS

The behaviour of the skewed puff with variable atmospheric stability is best illustrated by examples. Three atmospheric conditions, stable, L = 100, neutral, L = ∞ and unstable, L = - 100 were selected and horizontal puff spread estimated using $\sigma_x = \sigma_y = 0.22\ u_*t$. The following initial values were selected: $z(0) = 0.01$ m and $\sigma_x(0) = \sigma_y(0) = .1$ m. The surface roughness z_o was taken equal to 0.1 cm and the surface stress u_* was assumed to be 0.2 m s^{-1}.

Using these values, the position of the clouds centroid $(\bar{X},\bar{Z})$ were evaluated from Eqs. (2.16) and (2.17) concurrently with the shape parameter q from Eqs. (2.13) and (2.14). Setting the shearing parameter F = 0.38, also the skewing parameter ζ was calculated concurrently on the basis of Eq. (3.13). The lateral shear and thereby ξ was on the other hand assumed to be zero.

The three-dimensional concentration distribution function Eq. (3.15) describing the skewed puff is thereby specified as function of the travel time t, and in Fig. 5 is at time $t = 100$ shown the iso-concentration curve going through the centroid $(\bar{x},\bar{z})$ for the three different stabilities considered. The intention with the five elipses drawn are to visualize the symmetry of the puff in horizontal planes at arbitrary height. When looked at from above, these elipses will, with $\sigma_x = \sigma_y$, be circles with centre position (x_c,y_c) given by $(\zeta\bar{z},o)$ and radius $r = \sigma_x \{2b^q(1-z/\bar{z})^q\}^{1/2}$.

When stability is changed from stable through neutral to unstable conditions, the example shows that the mean height $\bar{z}$ of the cloud at fixed time increases, at the same time at the shape parameter q decreases. It is also evident from the figure that the contribution from the wind shear effect to the total horizontal spread Σ_x in this example is dominating over the spread at fixed height σ_x for all the three different stabilities considered. It can be concluded from the example that the spread σ_x yields a significant contribution to Σ_x only in a very unstable atmosphere.

The example seems also to suggest that the quantity Σ_x is approximatively constant over a broad range of stability around neutral. The specific results of the example is given in Tabel 1.

TABEL 1

Example in Fig. 5 with $u_* = 0.2\ ms^{-1}$, $z_o = 0.01$ m. T = 100 s

STABI-LITY	SKEWING PARAMETER	MEAN WIND SPEED (10 m)	MEAN ALONG WIND DISTANCE	MEAN HEIGHT	FIXED HEIGHT ALONG WIND SPREAD	TOTAL ALONG WIND SPREAD	TOTAL VERTICAL SPREAD	SHAPE PARA-METER
L[m]	ζ	$\bar{u}_{10}[ms^{-1}]$	$\bar{x}$[m]	$\bar{z}$[m]	σ_x[m]	Σ_x[m]	Σ_z[m]	q
100	4.40	4.84	462	9.1	5.2	77.5	17.6	1.37
∞	2.73	4.61	457	11.8	9.7	63.0	22.8	1.00
-100	1.82	4.47	453	15.0	9.9	53.0	28.8	0.65

5. CONCLUSION

A model for the spread of a ground level released puff of passive contaminant in a diabatic stratified surface layer has been developed for use in prediction of pollutant concentration in connection with a numerical puff model, where a serie of puffs are emitted successively from the source.

The following three-dimensional, normalized concentration distribution function of individual puffs have been proposed

$$C(\tilde{x},\tilde{y},\tilde{z}) =$$

$$\frac{a}{2\pi\sigma_x\sigma_y\bar{z}} \exp[-\tfrac{1}{2}(\tilde{x}-\zeta\tilde{z})^2/\sigma_x^2 - \tfrac{1}{2}(\tilde{y}-\xi\tilde{z})^2 - \left(\frac{b\tilde{z}}{\bar{z}}\right)^q] \tag{5.1}$$

where the two parameters (ζ,ξ) accounts for the shearing effect of the vertical wind velocity gradient. Their value are calculated by tagging the position of two tracer particles, z_1 and z_2, displaced by the distance $F\bar{z}$ about the mean height $\bar{z}$. The value of the constant F have been determined (0.38) in order that the total horizontal spread of the cloud equals theoretical predictions of the spread that results as a consequence of the interaction of shear and vertical diffusivity under neutral and very stable atmospheric conditions. The vertical concentration distribution

$$C_v(\tilde{z}) = \iint C(\tilde{x},\tilde{y},\tilde{z})d\tilde{x}d\tilde{y} = a/\bar{z}\,\exp(-b\tilde{z}/\bar{z})^q\ , \tag{5.2}$$

which is known to satisfy the diffusion equation exactly with a power law representation of the vertical eddy diffusivity, has from numerical solutions of the diffusion equation (2.7) been shown to be applicable also, when $\bar{z}$ is determined by the approximation

$$\frac{d\bar{z}}{dt} = K_z(\bar{z}/L)/\bar{z} \tag{5.3}$$

and the shape parameter q is determined by

$$q = 2 - d\log K_z/d\log z \qquad \text{for } z=\bar{z} \tag{5.4}$$

A numerical example seems to indicate that the total horizontal spread of the cloud Σ_x, at the fixed travel time t = 100 s, approximatively is constant over a broad range of the atmospheric stability. In contrast, the mean height $\bar{z}$ and the clouds shape parameter q are found to be strongly influenced by changes in the atmospheric stability.

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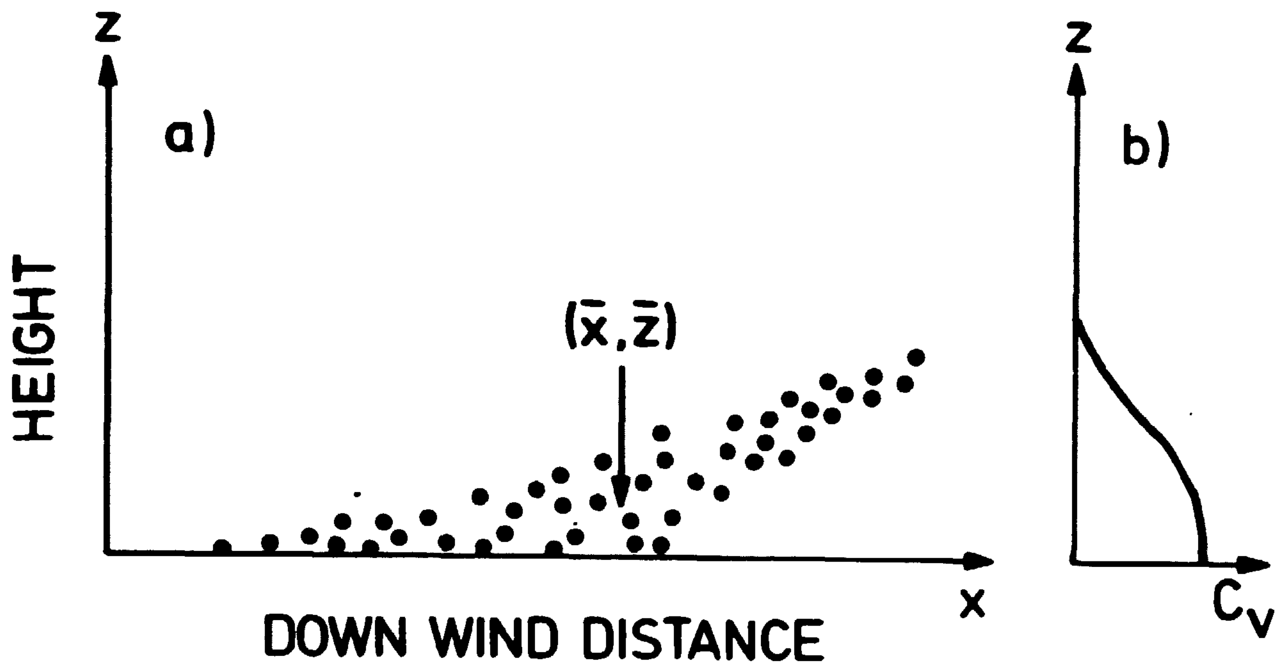


Fig. 1.
a) Diffusion of a number of particles released at x=0 at time t=0. The instantaneous position of the centre of mass of the cloud $(\bar{x},\bar{z})$ is indicated by the head of the arrow.
b) The corresponding instantaneous vertical particle distribution $C_V(z,t)$.

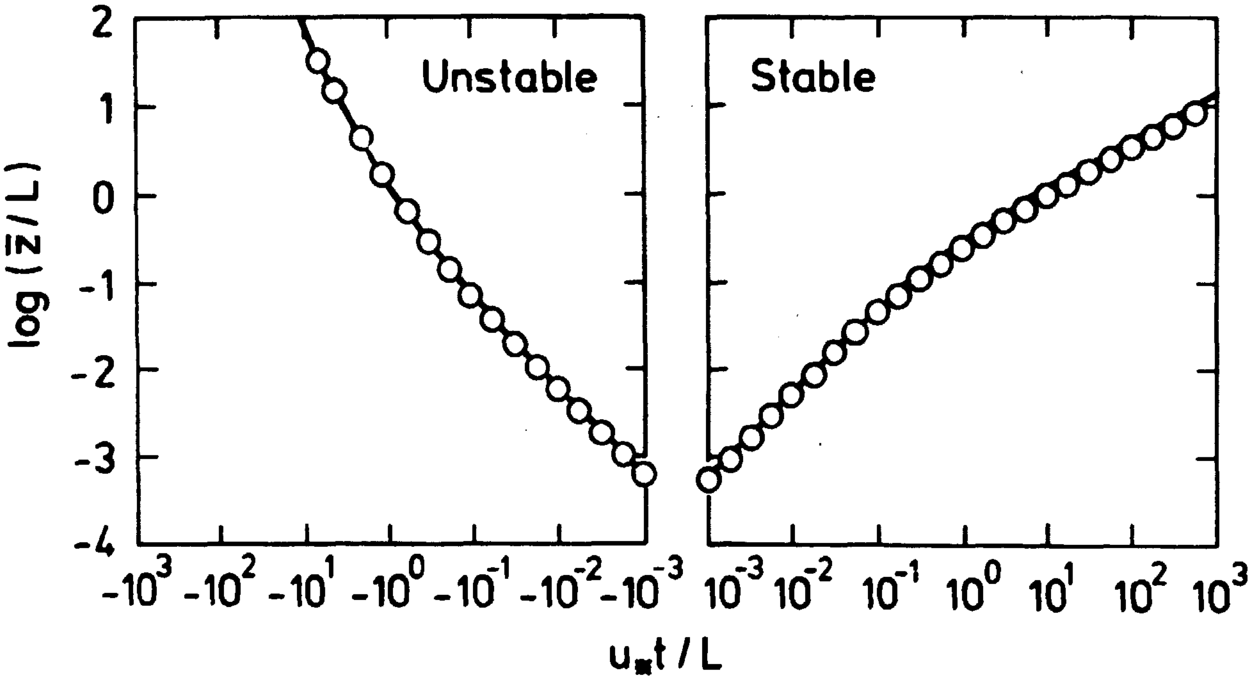
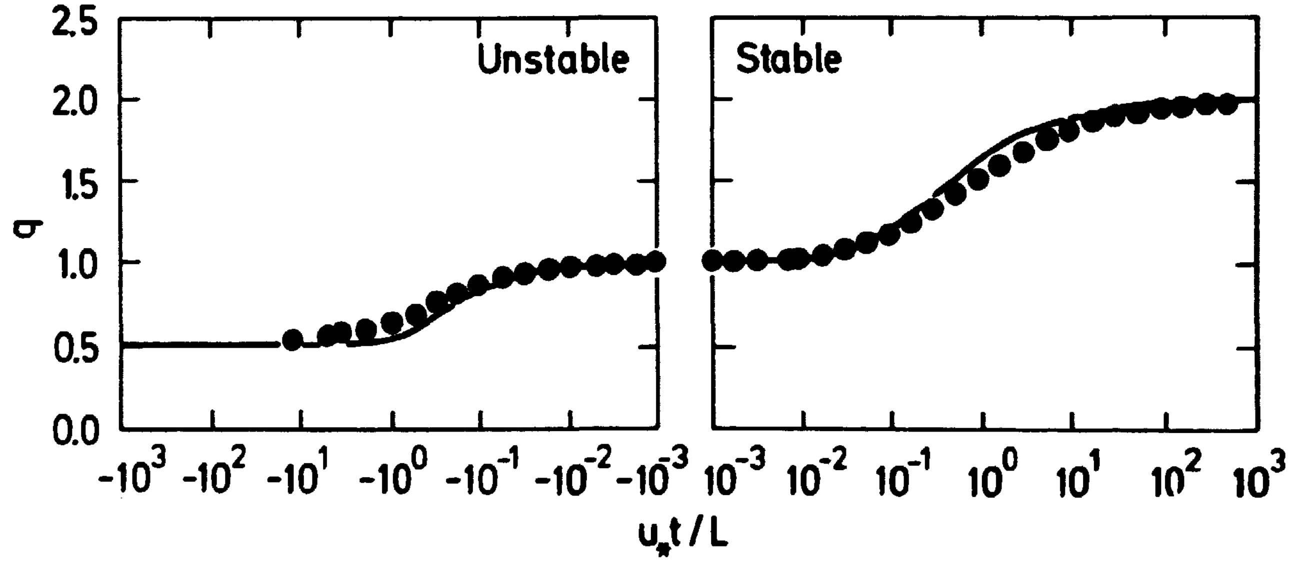
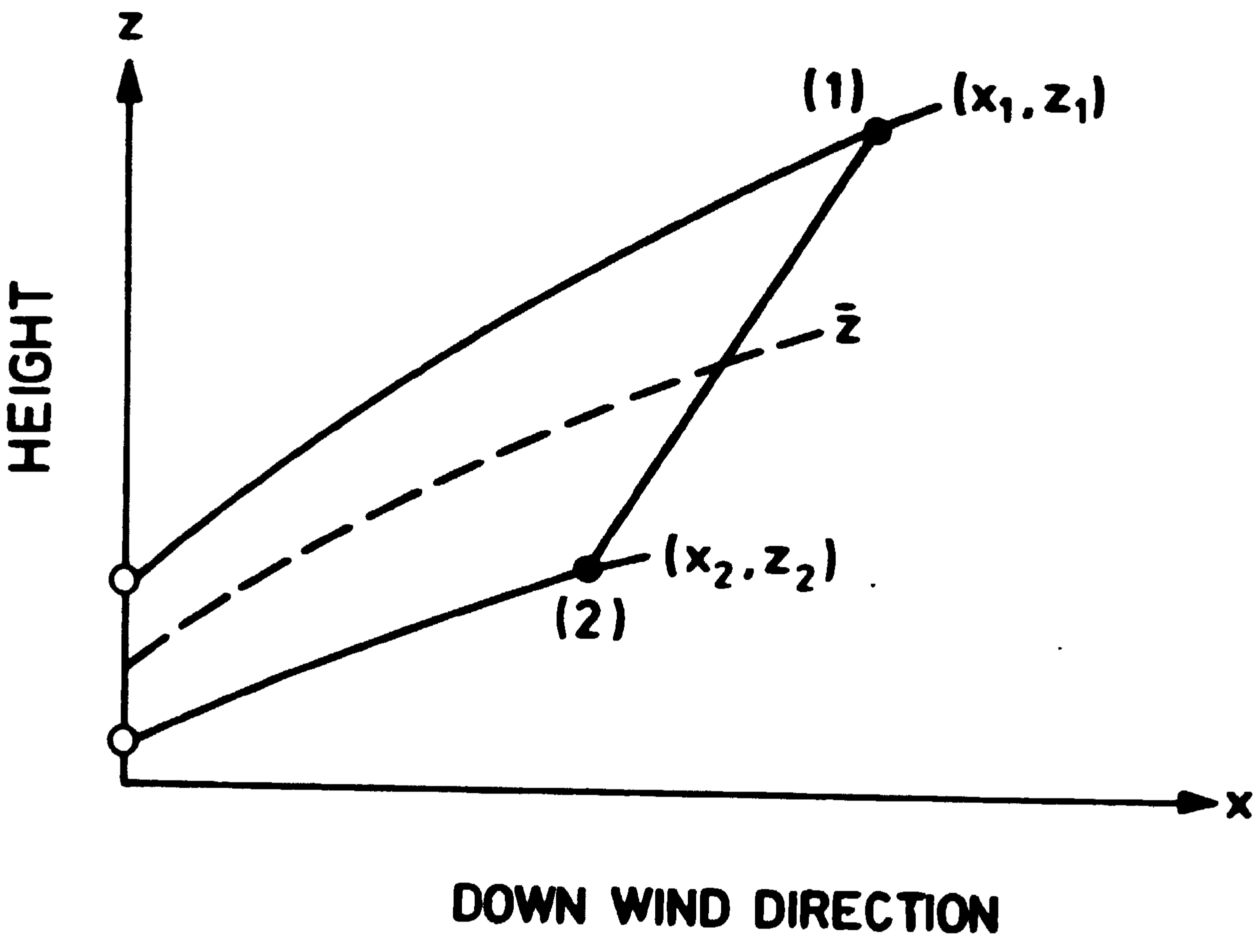


Fig. 2.
Dimensionless mean puff height $\bar{z}/L$ as function of the dimensionless travel time u_*t/L. The curve shows the approximation suggested in Eq. (2.16). The open circles represents the result of the numerical solution of the diffusion equation (2.24), together with the definition of $\bar{z}$, Eq. (2.4).



<u>Fig. 3.</u>

The shape factor q, as function of non-dimensional travel time u_*t/L. The curves show the analytical approximation suggested in Eq. (2.13) and (2.14). Dots represent least-square fitting of the analytical function described by Eq. (2.9) to C_y obtained from the numerical solution of Eq. (2.24).



<u>Fig. 4.</u>
Two tracer particles (1) and (2) displaced vertically by a constant fraction $F = (z_1-z_2)/2\bar{z}$ of the clouds mean height $\bar{z}$.

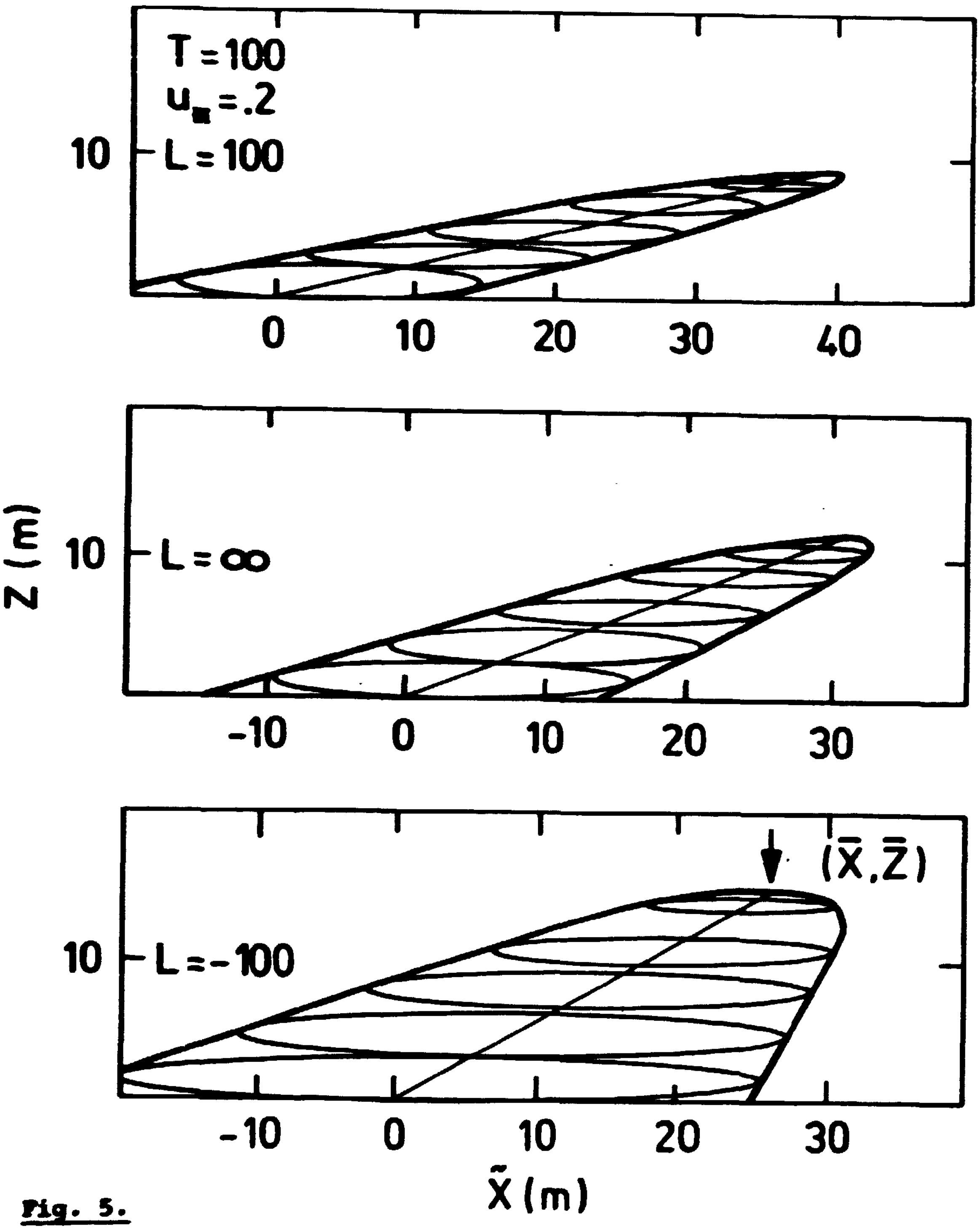


Fig. 5.

Skewed puff at t = 100 s for three atmospheric conditions: stable (L=100), neutral (L=) and unstable (L = - 100). Solid line shows the iso-concentration curve going through the centroid ($\bar{x}$,$\bar{z}$) in the vertical plane at y=0. The five circles in each plot are drawn to envision the extension of the iso-concentration curve into the cross wind direction. Reference on the abscissa is to the coordinate system $\tilde{x}$ moving with the base of the cloud, as defined in Eq. (3.4) and z is the height above the ground.

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A parametric description of a skewed puff in the diabatic surface layer

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Physics Dept.

Group's own registration number(s)

37 pages + tables + illustrations

Abstract

The spreading of passive material in the stable, neutral and unstable surface layer from an instantaneous ground source is parameterized in a form appropriate for use with an operational puff diffusion model.

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